1. A method for designing anti-tumor compositions, comprising:

(a) using molecular modeling software on a computer to create a plot of an active conformation of a known anti-tumor composition, said active conformation representative of a three-dimensional conformation of said known anti-tumor composition interacting with a target biological site, said plot providing a first digital representation of said active conformation, said first digital representation depicting a plurality of binding sites of said known anti-tumor composition;

(b) using said software to eliminate portions of said first digital representation while preserving the depiction of said binding sites;

(c) using said software to build a second digital representation of a created composition, said created composition having a three-dimensional conformation and binding sites similar to said known anti-tumor composition.

2. The method of Claim 1, wherein said known anti-tumor composition has a structure including a central skeleton which is depicted in said plot, and wherein said software is utilized to eliminate said central skeleton from said depiction and to substitute therefore a second central skeleton having desired characteristics.

3. The method of Claim 1, wherein said known anti-tumor composition has a structure including a central skeleton and one or more original side chains which are depicted in said plot, and wherein said software is utilized to eliminate one or more original side chains from said depiction and optionally to substitute a created side chain for one or more of said original side chains.

4. The method of Claim 3, further comprising using said software to eliminate said central skeleton from said depiction and to substitute therefore a second central skeleton having desired characteristics.

5. The method of Claims 1,2, 3 or 4 wherein a calculation is performed to determine a binding energy for said created composition, and wherein said created composition is further modified to improve putative binding characteristics, wherein an improved binding characteristic is characterized by a higher binding energy.

A1

6. The method of Claims 1, 2, 3 or 4, wherein said known anti-tumor composition is paclitaxel.

7. A method for designing a paclitaxel alternative composition, which alternative composition has a central skeleton structure composed of single or multiple ring groups which hold multiple functional groups in a fairly rigid alignment, said central skeleton structure having first, second, and third side chains;

wherein said first side chain is connected to said central skeleton with a carbonyl group at a distance of about 1.5 to 5.5 Angstroms from said central skeleton;

wherein said second side chain places an sp^3 oxygen atom at a distance of about 4.5 to 7.5 Angstroms from the skeleton and about 9 to 11 Angstroms from the carbonyl oxygen of said first side chain;

wherein said third side chain is placed in an energetically accessible conformation that places an aromatic ring in a location that is simultaneously about 4 to 6 Angstroms from a substitute for hexene and about 8 to 10 Angstroms from the oxygen in said second side chain, said third side chain selected to mimic the steric and binding properties of the C2 ester in paclitaxel;

said method comprising using molecular modeling software on a computer to design said alternative composition.

8. The method of Claim 7, wherein said alternative composition further comprises one or more bulking groups and wherein said bulking groups increase the size of said composition to mimic the overall size and shape of the paclitaxel molecule.

9. The method of Claim 7, wherein said first side chain is selected and positioned to mimic the isoserine group in taxane.

10. The method of Claim 7, wherein said sp^3 oxygen is positioned in space to simulate the position of the oxetane ring of paclitaxel.

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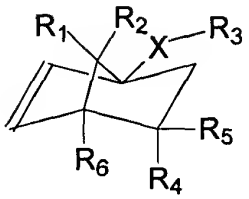
11. The method of Claims 7, 8, 9 or10, further comprising synthesizing said alternative composition.

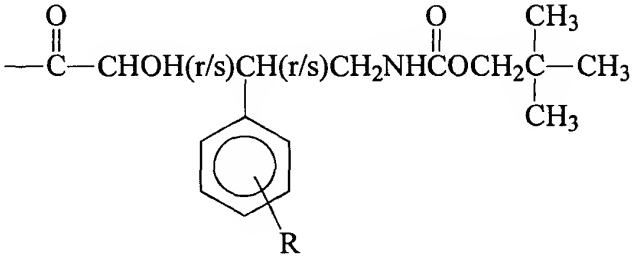
12. A paclitaxel compound having a chemical structure

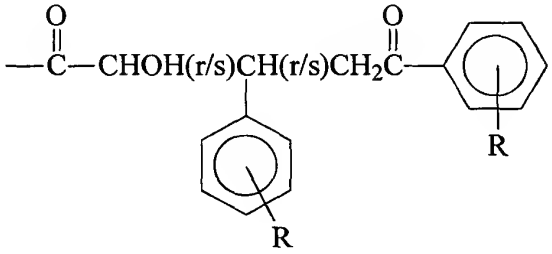


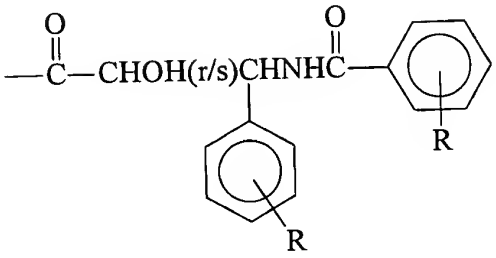
wherein R_1 and R_2 are selected from the group consisting of: hydrogen, methyl, acetyl, ethyl, C_1 - C_4 aliphatic chain and substituted C_1 - C_6 aliphatic chain, wherein said substituted aliphatic chain is substituted once or twice with functional groups selected from the group consisting of: amide, ketone, hydroxy, phenyl, carboxylic acid, and an amino acid;

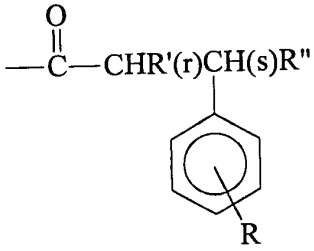
wherein X is selected from the group consisting of: O; CH_2; NH; S; S-CH_2; O-CH_2; or none;

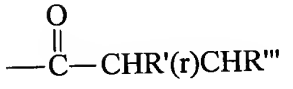
wherein R_3 is selected from the group consisting of:











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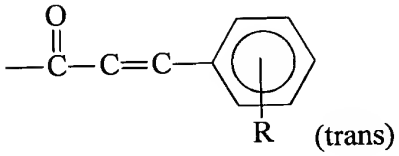

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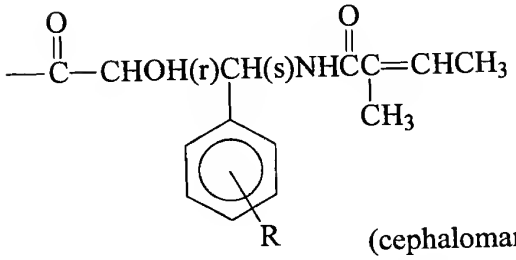
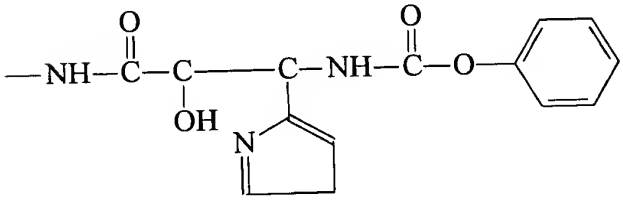
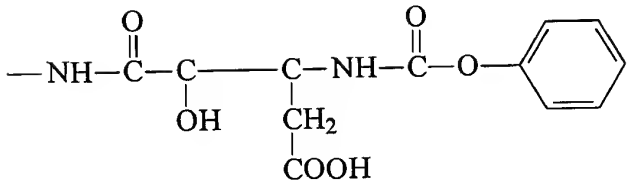
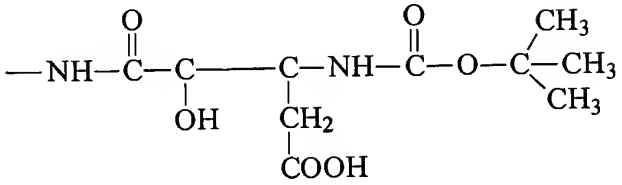
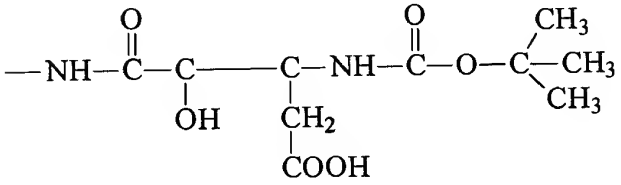


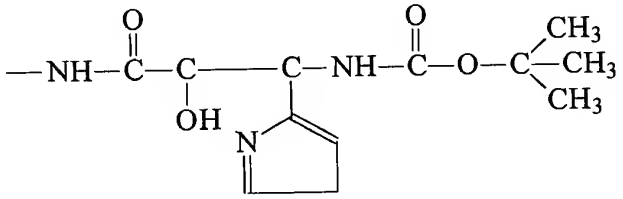
(cephalomannine)





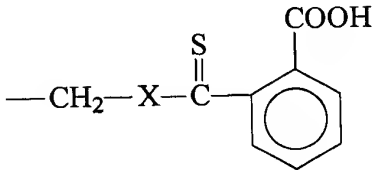


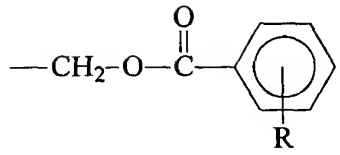


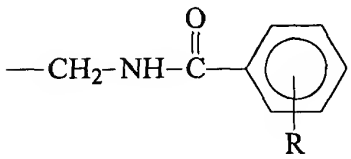


wherein the aryl rings are unsubstituted or singly, doubly, or triply substituted with R selected from the group consisting of: H, OH, and an electron withdrawing substituent;wherein R' is selected from the group consisting of: OH and H; wherein R" is selected from the group consisting of: NHBOC and H; wherein R"' is selected from the group consisting of: singly or doubly substituted aryl and fused aromatic ring;

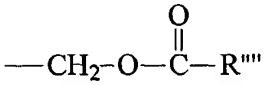
wherein R_4 is selected from the group consisting of:



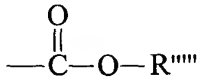




wherein the aromatic ring is singly, doubly, or triply substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

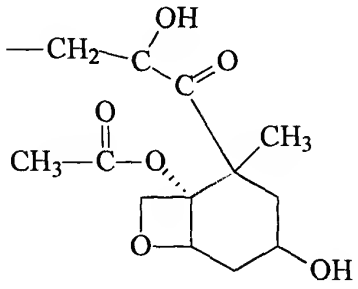


wherein R"" is a fixed aromatic ring or a fused aromatic ring substituted any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

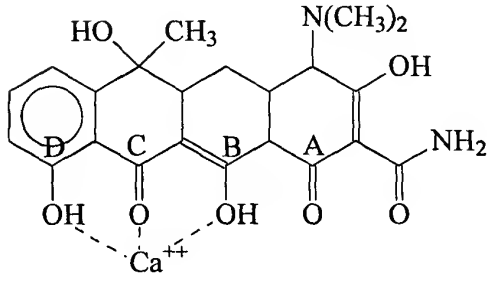


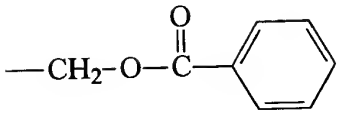
wherein R"" is selected from the group consisting of: H, cyclopropane, C_1-C_3 hydrocarbon chain, and C_1-C_3 substituted hydrocarbon chain wherein said substituted hydrocarbon chain is substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

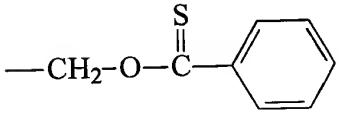
wherein R_5 is selected from the group consisting of:

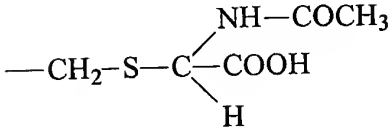


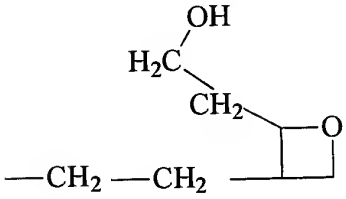
H, CH_3, C_1-C_5 hydrocarbon chain, C_1-C_5 substituted hydrocarbon chain, small hydrocarbon ring or heterocyclic ring, small substituted hydrocarbon ring or heterocyclic ring, citric acid and derivatives thereof, acetic acid and derivatives thereof, ascorbic acid and derivatives thereof, glucouroic acid or derivatives thereof, lactose, sialic acid, monosaccharides or disaccharides of glyceraldehyde, erythrose, threose, ribose, arabinose xylose lyxose, allose, altrose, glucose, mannose, gulose, idose, galactose, talose, or their acidic ketose, alditol or inositol forms, calcium chelating molecule, oxygenated small molecule, any organic molecule that exhibits calcium-binding properties similar to tetracyclin

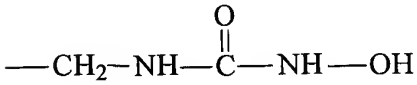












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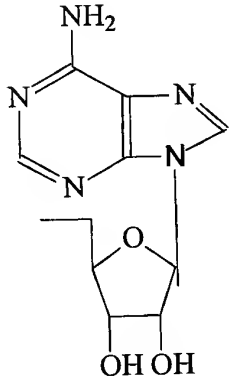
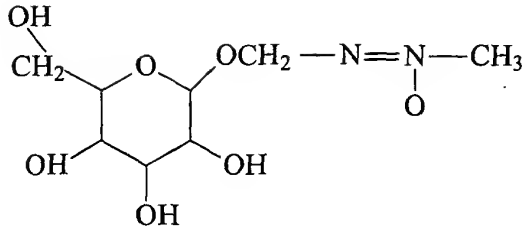
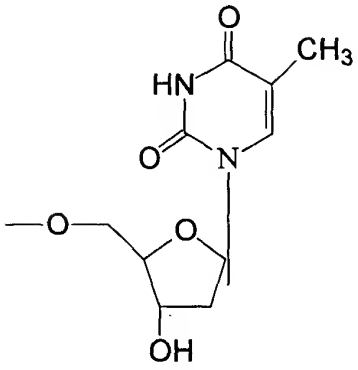
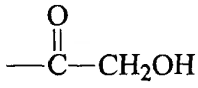
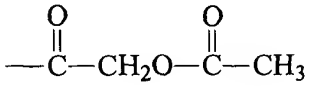


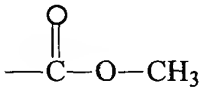




wherein R_6 is selected from the group consisting of:

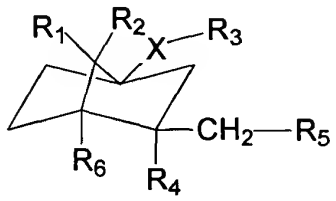






H, CH_3, OH, amine, C_1-C_5 carbo-aliphatic chain substituted with two or three of the following groups selected from the group consisting of: keto, hydroxy, sulfoxy, amide, an amino acid, and ethers of the form -CH_2-O-$(CH_2)_n$-CH_3 where n=1-5, wherein the right hand hydrocarbon chain is unsubstituted or substituted with 1 to 5 -OH or carbonyl groups.

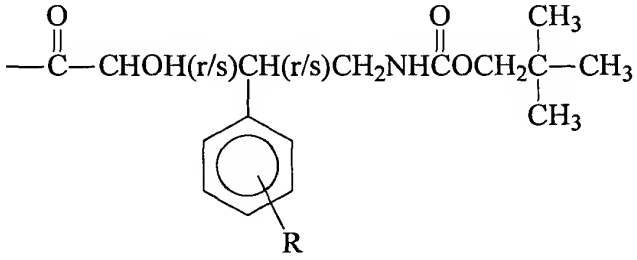
13. A paclitaxel compound having a chemical structure

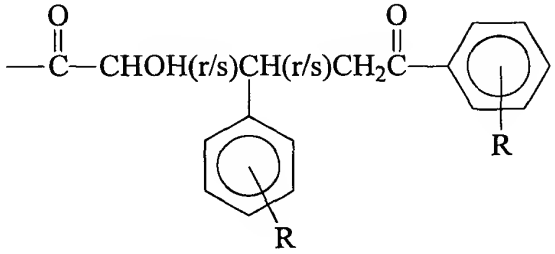


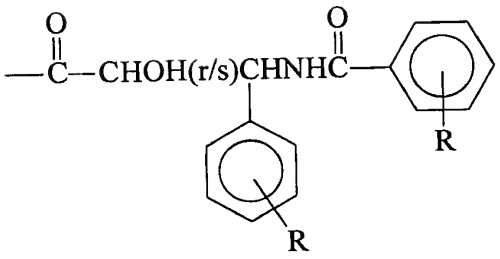
wherein R_1 and R_2 are selected from the group consisting of: hydrogen, methyl, acetyl, ethyl, C_1 - C_4 aliphatic chain and substituted C_1 - C_6 aliphatic chain, wherein said substituted aliphatic chain is substituted once or twice with functional groups selected from the group consisting of: amide, ketone, hydroxy, phenyl, carboxylic acid, and an amino acid;

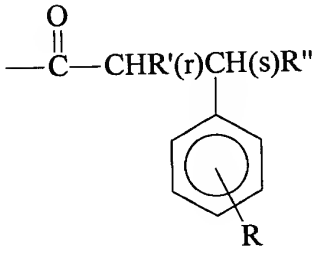
wherein X is selected from the group consisting of: O; CH_2; NH; S; S-CH_2; O-CH_2; or none;

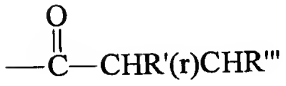
wherein R_3 is selected from the group consisting of:











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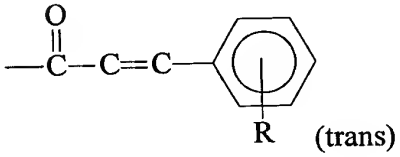

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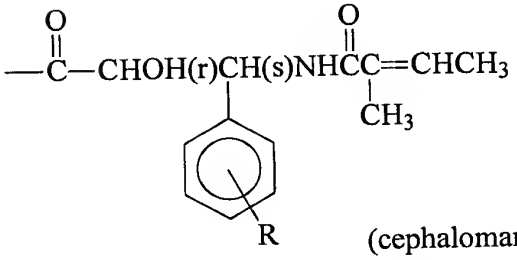

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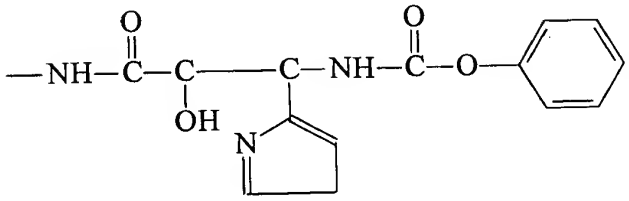
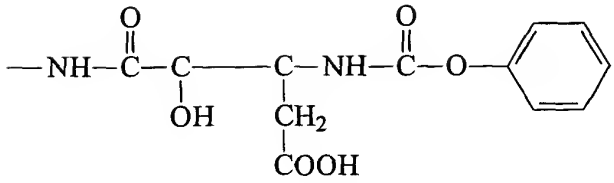
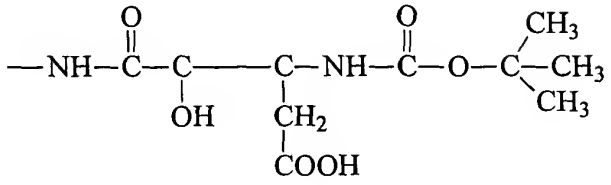
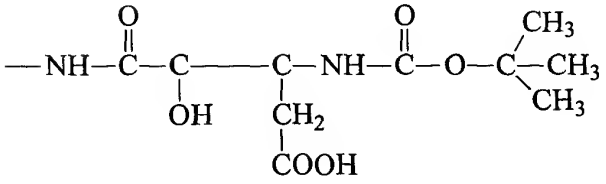
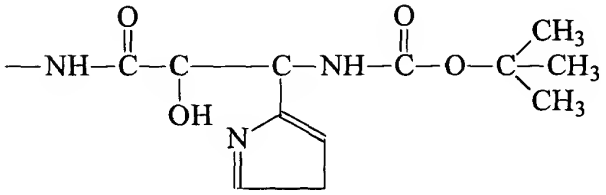




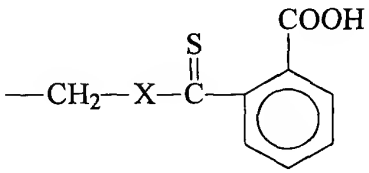


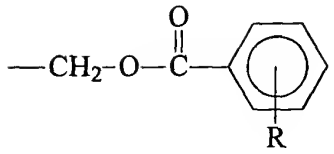


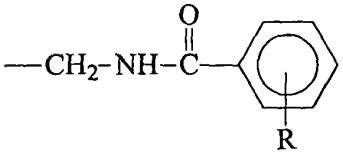


wherein the aryl rings are unsubstituted or singly, doubly, or triply substituted with R selected from the group consisting of: H, OH, and an electron withdrawing substituent; wherein R' is selected from the group consisting of: OH and H; wherein R" is selected from the group consisting of: NHBOC and H; wherein R"' is selected from the group consisting of: singly or doubly substituted aryl and fused aromatic ring;

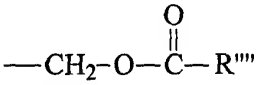
wherein R_4 is selected from the group consisting of:



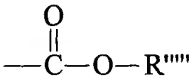




wherein the aromatic ring is singly, doubly, or triply substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

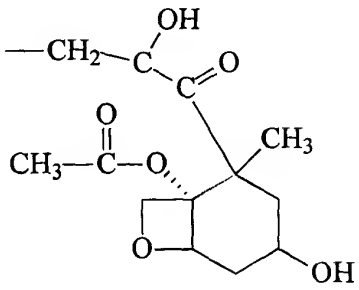


wherein R"" is a fixed aromatic ring or a fused aromatic ring substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

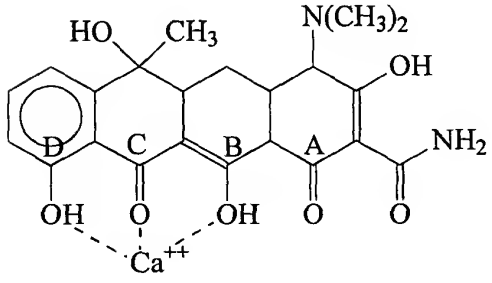


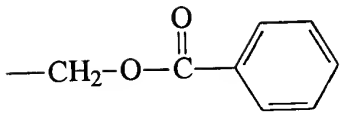
wherein R"" is selected from the group consisting of: H, cyclopropane, C_1-C_3 hydrocarbon chain, and C_1-C_3 substituted hydrocarbon chain wherein said substituted hydrocarbon chain is substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

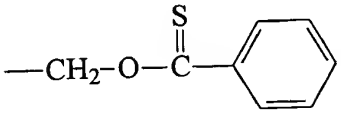
wherein R_5 is selected from the group consisting of:

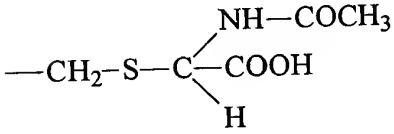


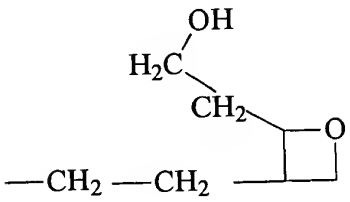
H, CH_3, C_1-C_5 hydrocarbon chain, C_1-C_5 substituted hydrocarbon chain, small hydrocarbon ring or heterocyclic ring, small substituted hydrocarbon ring or heterocyclic ring, citric acid and derivatives thereof, acetic acid and derivatives thereof, ascorbic acid and derivatives thereof, glucouroic acid or derivatives thereof, lactose, sialic acid, monosaccharides or disaccharides of glyceraldehyde, erythrose, threose, ribose, arabinose xylose lyxose, allose, altrose, glucose, mannose, gulose, idose, galactose, talose, or their acidic ketose, alditol or inositol forms, calcium chelating molecule, oxygenated small molecule, any organic molecule that exhibits calcium-binding properties similar to tetracyclin

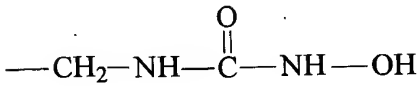












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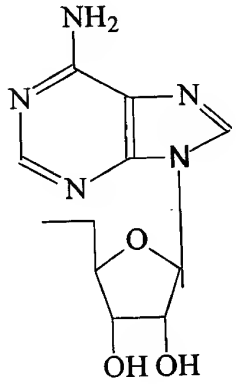
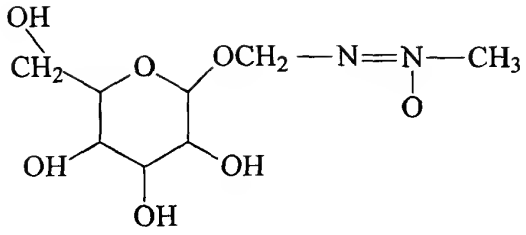
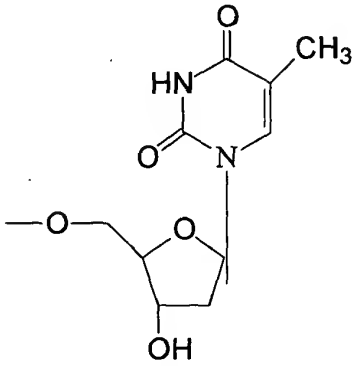
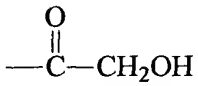
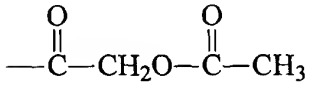


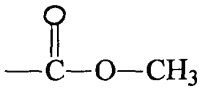




wherein R_6 is selected from the group consisting of:



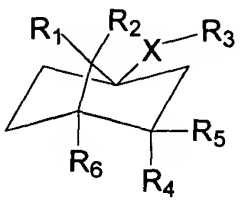




H, CH_3, OH, amine, C_1-C_5 carbo-aliphatic chain substituted with two or three of the following groups selected from the group consisting of: keto, hydroxy, sulfoxy, amide, an amino acid, ethers of the form $-CH_2-O-(CH_2)_n-CH_3$ where n=1-5, wherein the right hand hydrocarbon chain is unsubstituted or substituted with 1 to 5 -OH or carbonyl groups.

A3

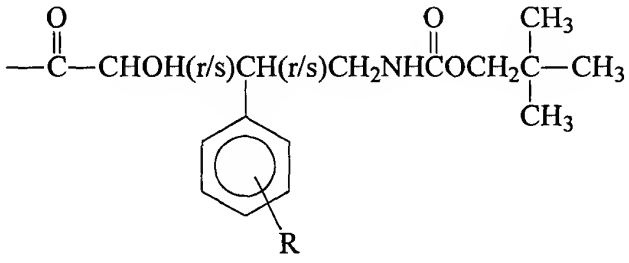
14. A paclitaxel compound having a chemical structure

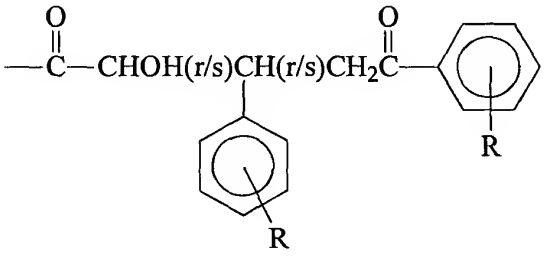


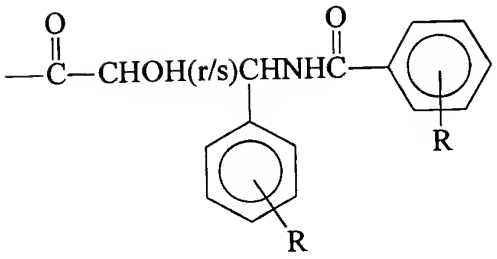
wherein R_1 and R_2 are selected from the group consisting of: hydrogen, methyl, acetyl, ethyl, C_1 - C_4 aliphatic chain and substituted C_1 - C_6 aliphatic chain, wherein said substituted aliphatic chain is substituted once or twice with functional groups selected from the group consisting of: amide, ketone, hydroxy, phenyl, carboxylic acid, and an amino acid;

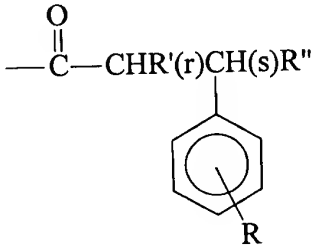
wherein X is selected from the group consisting of: O; CH_2; NH; S; S-CH_2; O-CH_2; or none;

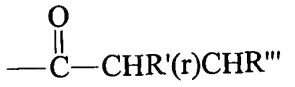
wherein R_3 is selected from the group consisting of:



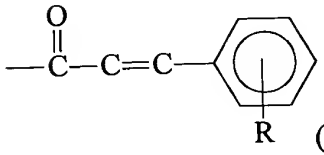


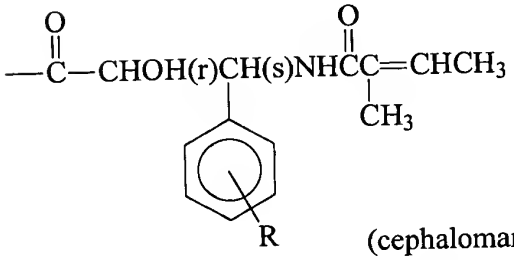


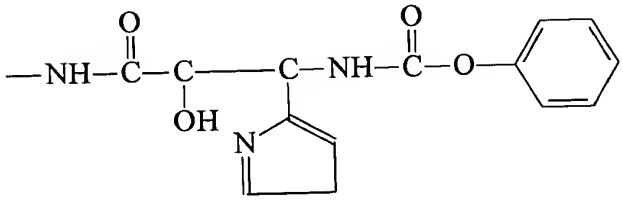


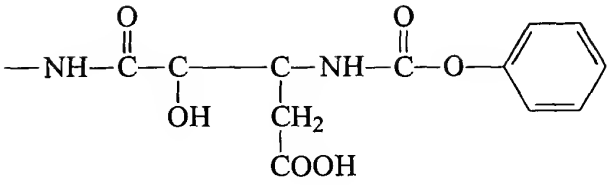


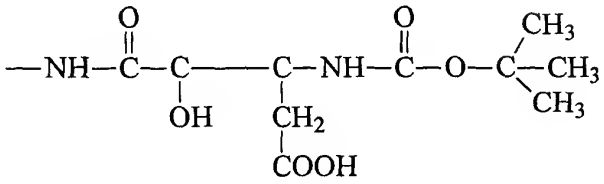
15

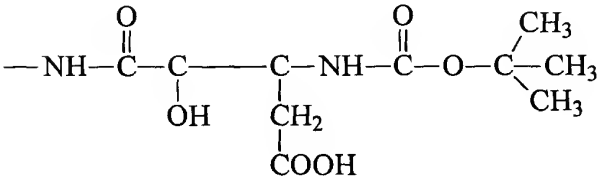

(trans)

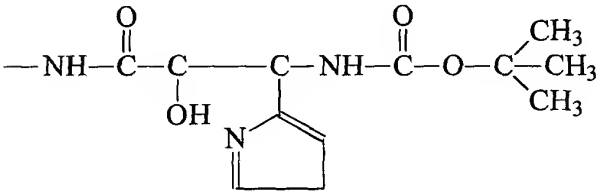

(cephalomannine)





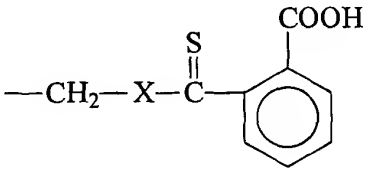


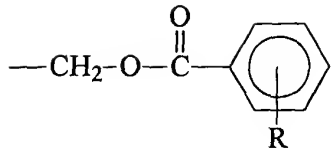


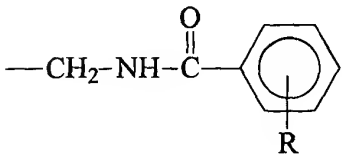


wherein the aryl rings are unsubstituted or singly, doubly, or triply substituted with R selected from the group consisting of: H, OH, and an electron withdrawing substituent;wherein R' is selected from the group consisting of: OH and H; wherein R" is selected from the group consisting of: NHBOC and H; wherein R"' is selected from the group consisting of: singly or doubly substituted aryl and fused aromatic ring;

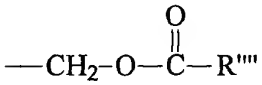
wherein R_4 is selected from the group consisting of:



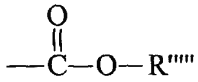




wherein the aromatic ring is singly, doubly, or triply substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;



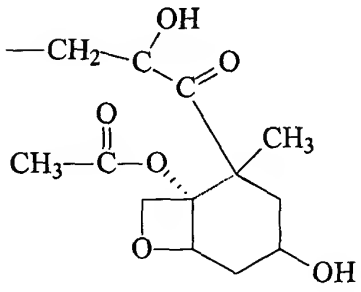
wherein R"" is a fixed aromatic ring or a fused aromatic ring substituted with R any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;



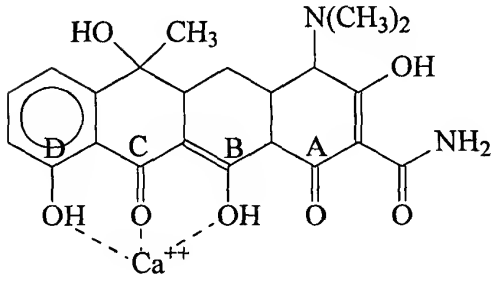
wherein R""" is selected from the group consisting of: H, cyclopropane, C_1-C_3 hydrocarbon chain, and C_1-C_3 substituted hydrocarbon chain wherein said substituted hydrocarbon chain is substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

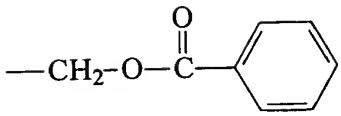
A3

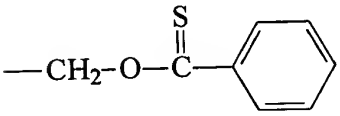
wherein R_5 is selected from the group consisting of:

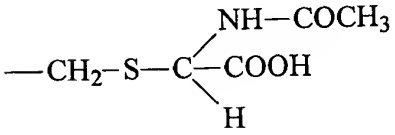


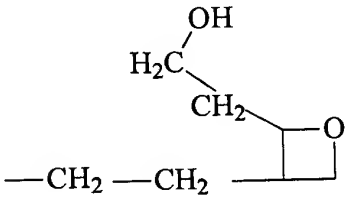
H, CH_3, C_1-C_5 hydrocarbon chain, C_1-C_5 substituted hydrocarbon chain, small hydrocarbon ring or heterocyclic ring, small substituted hydrocarbon ring or heterocyclic ring, citric acid and derivatives thereof, acetic acid and derivatives thereof, ascorbic acid and derivatives thereof, glucouroic acid or derivatives thereof, lactose, sialic acid, monosaccharides or disaccharides of glyceraldehyde, erythrose, threose, ribose, arabinose xylose lyxose, allose, altrose, glucose, mannose, gulose, idose, galactose, talose, or their acidic ketose, alditol or inositol forms, calcium chelating molecule, oxygenated small molecule, any organic molecule that exhibits calcium-binding properties similar to tetracyclin

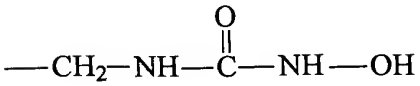












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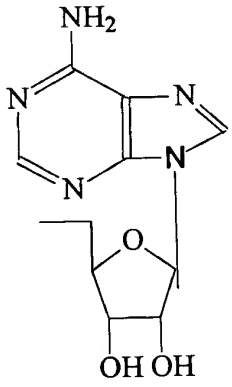
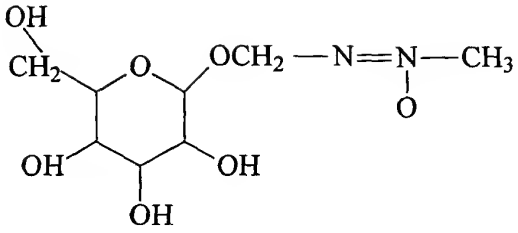
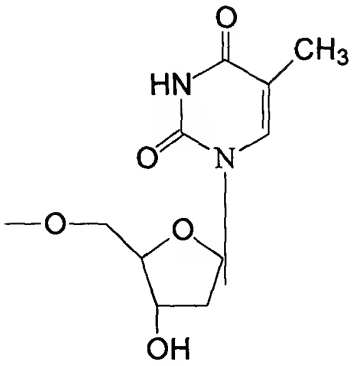
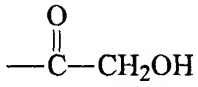


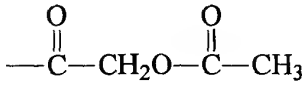
A3

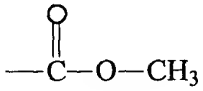




wherein R_6 is selected from the group consisting of:

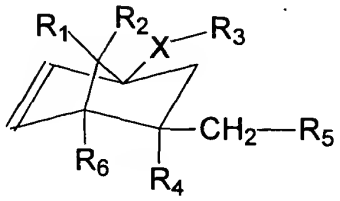






H, CH_3, OH, amine, C_1-C_5 carbo-aliphatic chain substituted with two or three of the following groups selected from the group consisting of: keto, hydroxy, sulfoxy, amide, an amino acid, ethers of the form $-CH_2-O-(CH_2)_n-CH_3$ where n=1-5, wherein the right hand hydrocarbon chain is unsubstituted or substituted with 1 to 5 -OH or carbonyl groups.

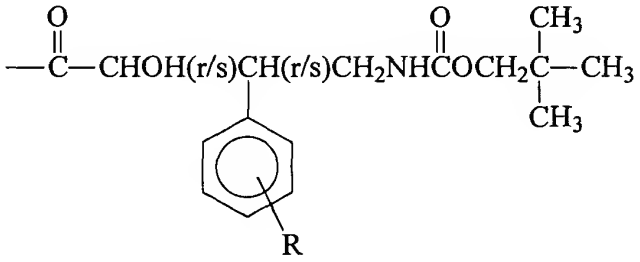
15. A paclitaxel compound having a chemical structure

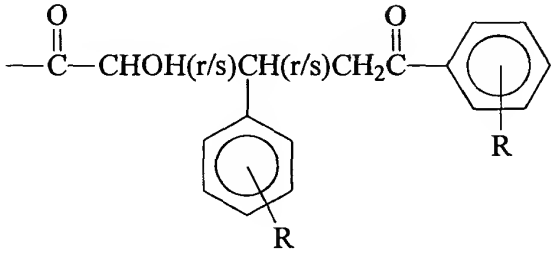


wherein R_1 and R_2 are selected from the group consisting of: hydrogen, methyl, acetyl, ethyl, C_1 - C_4 aliphatic chain and substituted C_1 - C_6 aliphatic chain, wherein said substituted aliphatic chain is substituted once or twice with functional groups selected from the group consisting of: amide, ketone, hydroxy, phenyl, carboxylic acid, and an amino acid;

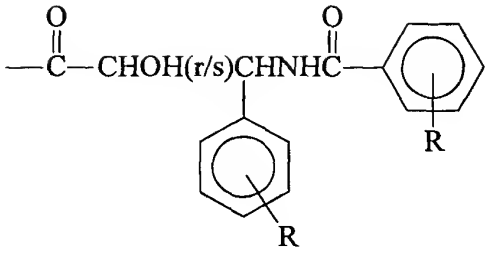
wherein X is selected from the group consisting of: O; CH_2; NH; S; S-CH_2; O-CH_2; or none;

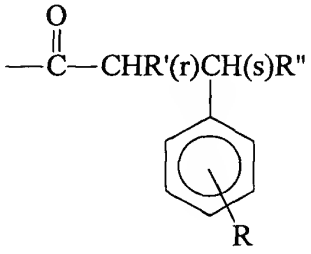
wherein R_3 is selected from the group consisting of:





A3





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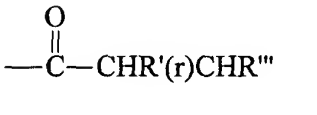
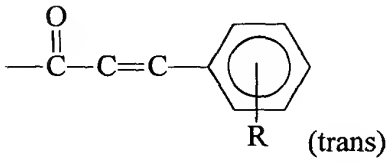
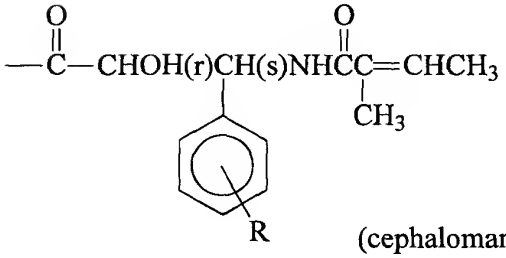
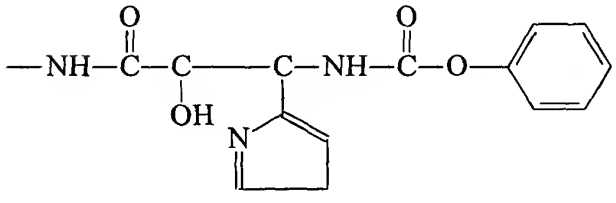
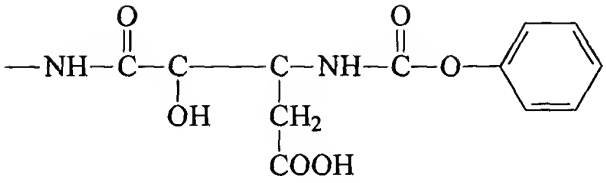
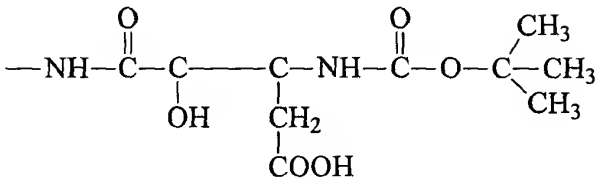


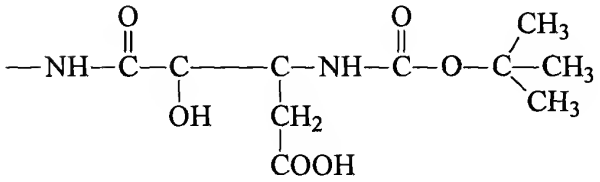


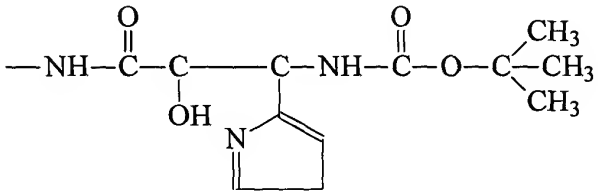






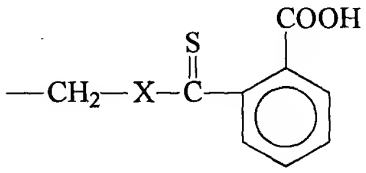


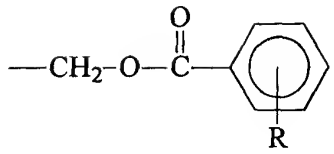


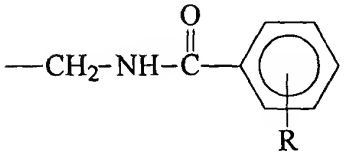


wherein the aryl rings are unsubstituted or singly, doubly, or triply substituted with R selected from the group consisting of: H, OH, and an electron withdrawing substituent;wherein R' is selected from the group consisting of: OH and H; wherein R" is selected from the group consisting of: NHBOC and H; wherein R"' is selected from the group consisting of: singly or doubly substituted aryl and fused aromatic ring;

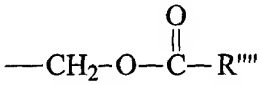
wherein R_4 is selected from the group consisting of:



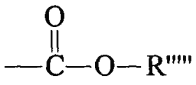




wherein the aromatic ring is singly, doubly, or triply substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

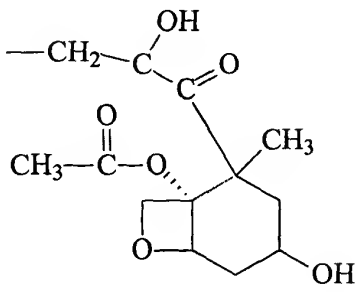


wherein R"" is a fixed aromatic ring or a fused aromatic ring substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

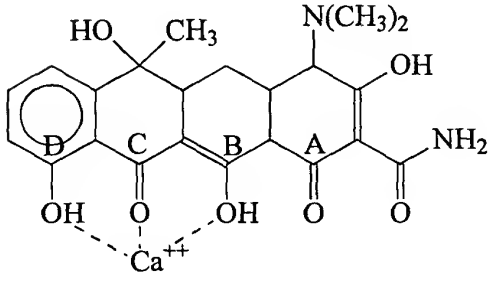


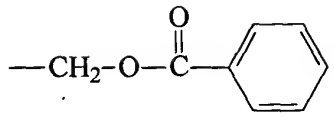
wherein R"" is selected from the group consisting of: H, cyclopropane, C_1-C_3 hydrocarbon chain, and C_1-C_3 substituted hydrocarbon chain wherein said substituted hydrocarbon chain is substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

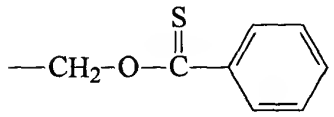
wherein R_5 is selected from the group consisting of:

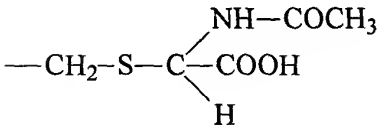


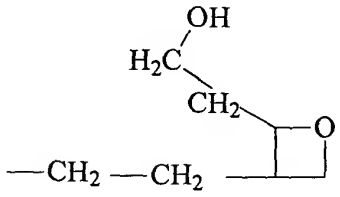
H, CH_3, C_1-C_5 hydrocarbon chain, C_1-C_5 substituted hydrocarbon chain, small hydrocarbon ring or heterocyclic ring, small substituted hydrocarbon ring or heterocyclic ring, citric acid and derivatives thereof, acetic acid and derivatives thereof, ascorbic acid and derivatives thereof, glucouroic acid or derivatives thereof, lactose, sialic acid, monosaccharides or disaccharides of glyceraldehyde, erythrose, threose, ribose, arabinose xylose lyxose, allose, altrose, glucose, mannose, gulose, idose, galactose, talose, or their acidic ketose, alditol or inositol forms, calcium chelating molecule, oxygenated small molecule, any organic molecule that exhibits calcium-binding properties similar to tetracyclin

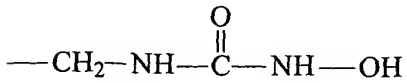












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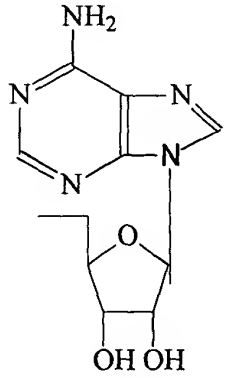
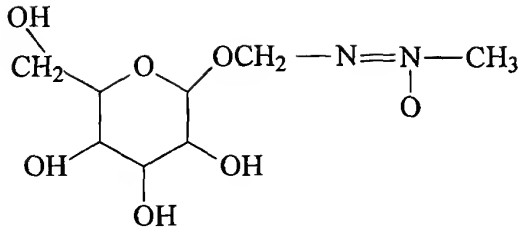
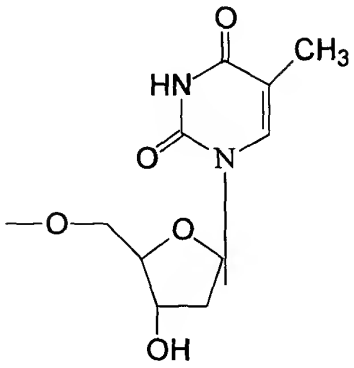
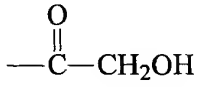


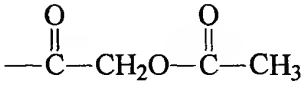
A3

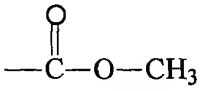




wherein R_6 is selected from the group consisting of:

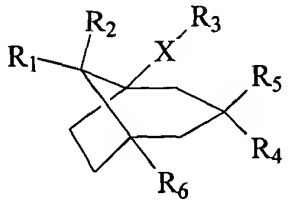






H, CH_3, OH, amine, C_1-C_5 carbo-aliphatic chain substituted with two or three of the following groups selected from the group consisting of: keto, hydroxy, sulfoxy, amide, an amino acid, ethers of the form $-CH_2-O-(CH_2)_n-CH_3$ where n=1-5, wherein the right hand hydrocarbon chain is unsubstituted or substituted with 1 to 5 -OH or carbonyl groups.

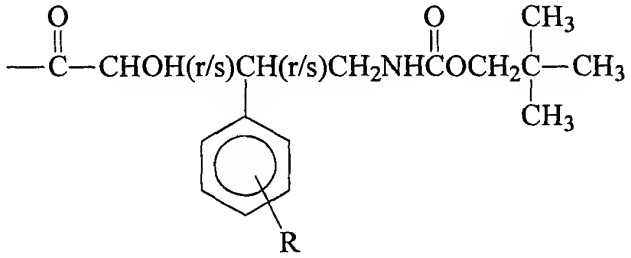
16. A paclitaxel compound having the following bicyclo-octane chemical structure

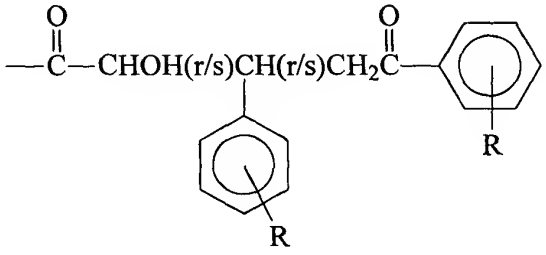


wherein R_1 and R_2 are selected from the group consisting of: hydrogen, methyl, acetyl, ethyl, C_1 - C_4 aliphatic chain and substituted C_1 - C_6 aliphatic chain, wherein said substituted aliphatic chain is substituted once or twice with functional groups selected from the group consisting of: amide, ketone, hydroxy, phenyl, carboxylic acid, and an amino acid;

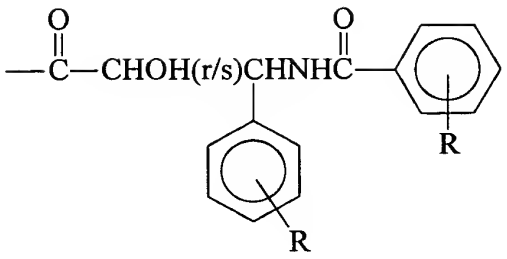
wherein X is selected from the group consisting of: O; CH_2; NH; S; S-CH_2; and O-CH_2;

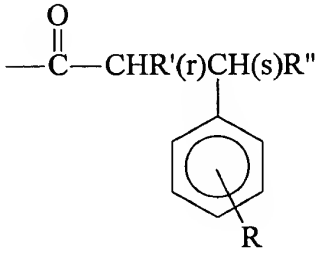
wherein R_3 is selected from the group consisting of:





A3





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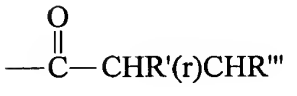
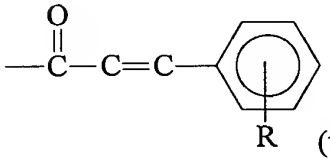
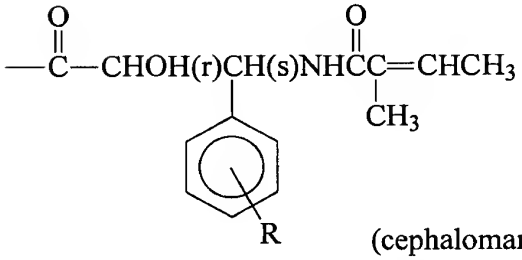
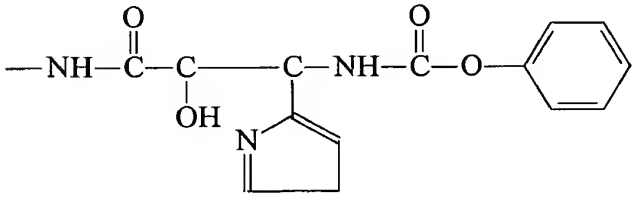
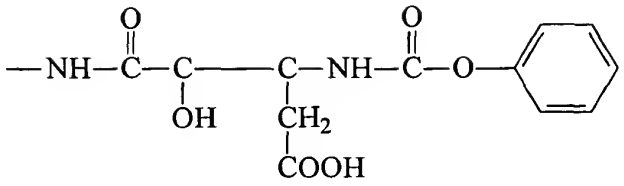
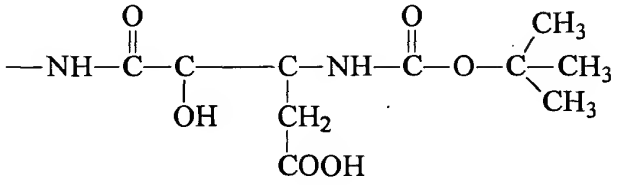


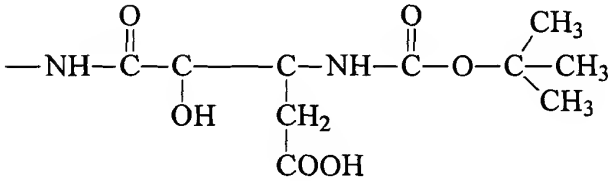


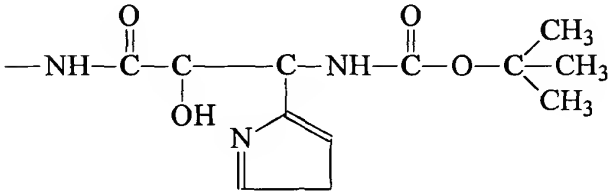






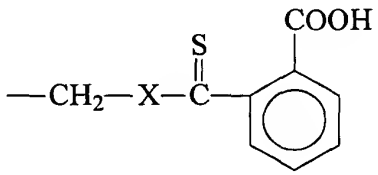




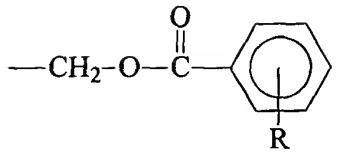


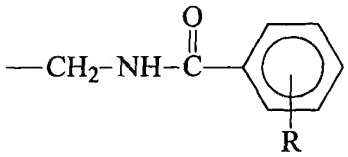
wherein the aryl rings are unsubstituted or singly, doubly, or triply substituted with R selected from the group consisting of: H, OH, and an electron withdrawing substituent; wherein R' is selected from the group consisting of: OH and H; wherein R" is selected from the group consisting of: NHBOC and H; wherein R"' is selected from the group consisting of: singly or doubly substituted aryl and fused aromatic ring;

wherein R_4 is selected from the group consisting of:

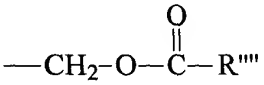


A3

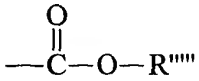




wherein the aromatic ring is singly, doubly, or triply substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;



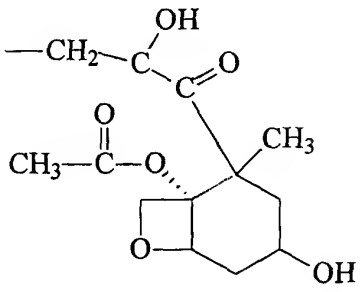
wherein R"" is a fixed aromatic ring or a fused aromatic ring substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;



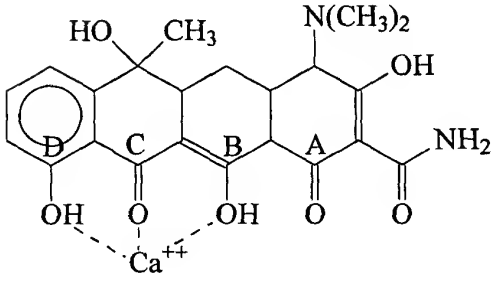
wherein R"" is selected from the group consisting of: H, cyclopropane, C_1-C_3 hydrocarbon chain, and C_1-C_3 substituted hydrocarbon chain wherein said substituted hydrocarbon chain is substituted with any electron-withdrawing substituent compatible with the system which provides a lower energy gap in a π - π interaction;

A3

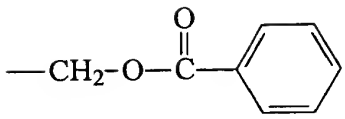
wherein R_5 is selected from the group consisting of:

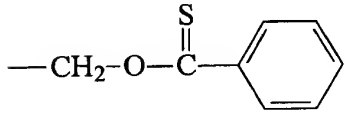


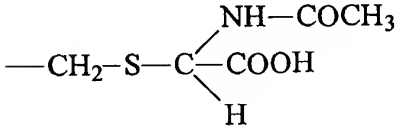
H, CH_3, C_1-C_5 hydrocarbon chain, C_1-C_5 substituted hydrocarbon chain, small hydrocarbon ring or heterocyclic ring, small substituted hydrocarbon ring or heterocyclic ring, citric acid and derivatives thereof, acetic acid and derivatives thereof, ascorbic acid and derivatives thereof, glucouroic acid or derivatives thereof, lactose, sialic acid, monosaccharides or disaccharides of glyceraldehyde, erythrose, threose, ribose, arabinose xylose lyxose, allose, altrose, glucose, mannose, gulose, idose, galactose, talose, or their acidic ketose, alditol or inositol forms, calcium chelating molecule, oxygenated small molecule, any organic molecule that exhibits calcium-binding properties similar to tetracyclin

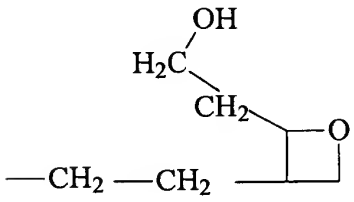


A3









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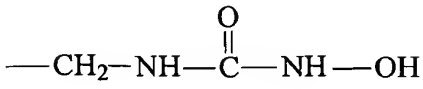

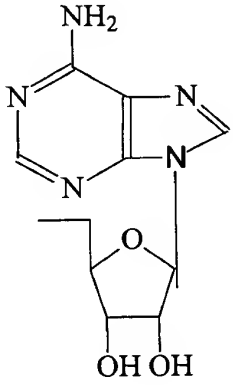

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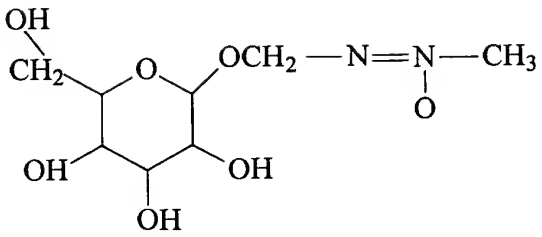
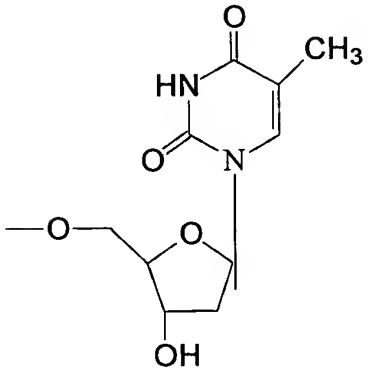
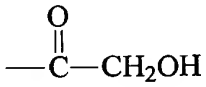
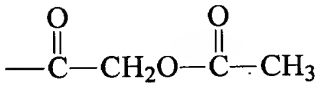
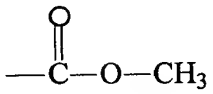




wherein R_6 is selected from the group consisting of:







H, CH_3;, OH, amine, C_1-C_5 carbo-aliphatic chain substituted with two or three of the following groups selected from the group consisting of: keto, hydroxy, sulfoxy, amide, an amino acid, ethers of the form $-CH_2-O-(CH_2)_n-CH_3$ where n=1-5, wherein the right hand hydrocarbon chain is unsubstituted or substituted with 1 to 5 -OH or carbonyl groups.

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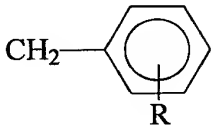
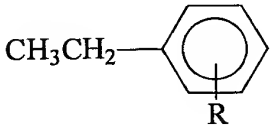
17. The compound of claim 12, 13, 14, 15, or 16, wherein the amino acid identity of R_1 or R_2 is selected from the group consisting of asparagine, glutamine, aspartic acid, glutamic acid, threonine, serine and tyrosine.

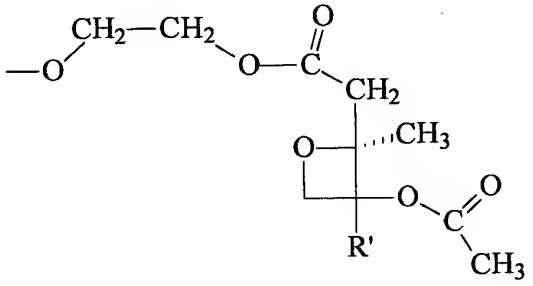
18. The compound of claim 12, 13, 14, 15, or 16, wherein R_1 is chosen from the group consisting of H and CH_3.

19. The compound of claim 12, 13, 14, 15, or 16, wherein R_2 is chosen from the group consisting of CH_3, CH_2OCOCH_3,





wherein R is H or singly, doubly, or triply substituted or fused; and



wherein R' is selected from the group consisting of H and CH_3.

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20. The compound of claim 12, 13, 14, 15, or 16, wherein R''' is selected from the group consisting of imidazol ring, tryptophan unsubstituted or substituted with carboxylic acid derivatives.

21. The compound of claim 12, 13, 14, 15, or 16, wherein R_3 is any group derived from the 13 position in taxane's skeleton that exhibits activity toward inhibiting the depolymerization of microtubules or anticancer activity.

22. The compound of claim 12, 13, 14, 15, or 16, wherein the oxygenated small molecule of R_5 is selected from the group consisting of dipeptides of "ASP-ASN", or "GLY-GLN" and the cyclic dipeptide of "PHE-GLN."

23. The compound of claim 12, 13, 14, 15, or 16, wherein the amino acid of R_6 is selected from the group consisting of serine, asparagine, and threonine.

A3 cont'd

24. The method of Claim 5, wherein said known anti-tumor composition is paclitaxel.